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A general framework of SVM in HDLSS settings

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1 Introduction

High-dimension, low-sample-size (HDLSS) data situations occur in many areas of modern science such as genetic microarrays, medical imaging, text recognition, finance, chemometrics, and so on. Suppose we have independent and d -variate two populations, Π_i , $i = 1, 2$, having an unknown mean vector $\boldsymbol{\mu}_i$ and unknown covariance matrix $\boldsymbol{\Sigma}_i$ for each i . We have independent and identically distributed (i.i.d.) observations, $\boldsymbol{x}_{i1}, \dots, \boldsymbol{x}_{in_i}$; from each Π_i . We assume $n_i \geq 2$, $i = 1, 2$. Let \boldsymbol{x}_0 be an observation vector of an individual belonging to one of the two populations. Let $N = n_1 + n_2$. We assume \boldsymbol{x}_0 and \boldsymbol{x}_{ij} s are independent.

In this paper, we consider classification in the HDLSS context such as $d \rightarrow \infty$ while N is fixed. In the HDLSS context, Hall et al. [6], Marron et al. [8] and Qiao et al. [12] considered distance weighted classifiers. Hall et al. [7], Chan and Hall [5] and Aoshima and Yata [2] considered distance-based classifiers. In particular, Aoshima and Yata [2] gave the misclassification rate adjusted classifier for multiclass, high-dimensional data in which misclassification rates are no more than specified thresholds. On the other hand, Aoshima and Yata [1, 3] considered geometric classifiers based on a geometric representation of HDLSS data. Aoshima and Yata [4] considered quadratic classifiers in general and discussed asymptotic properties and optimality of the classifiers under high-dimension, non-sparse settings. For linear SVM in HDLSS settings, Hall et al. [6], Chan and Hall [5] and Qiao and Zhang [13] showed that the misclassification rates tend to zero as $d \rightarrow \infty$ under certain severe conditions. Nakayama et al. [9] investigated asymptotic properties of linear SVM for HDLSS data. They proposed

a bias-corrected linear SVM and showed that it gives preferable performances compared to linear SVM. On the other hand, Nakayama et al. [10] investigated asymptotic properties of SVM with the Gaussian kernel for HDLSS data.

In this paper, we consider a general framework of SVM in the HDLSS context where $d \rightarrow \infty$ while N is fixed. In Section 2, we investigate asymptotic properties of SVM in the HDLSS. In Section 3, we give asymptotic properties of SVM for both the linear and the Gaussian kernels.

2 A general framework of SVM

In this section, we consider a general framework of SVM.

2.1 Setup of SVM

Since HDLSS data are mostly separable by a hyperplane, we consider the hard-margin SVM as follows:

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b, \quad (1)$$

where $\phi(\cdot)$ is a feature map, \mathbf{w} is a weight vector and b is an intercept term. Let us write that $(\mathbf{x}_1, \dots, \mathbf{x}_N) = (\mathbf{x}_{11}, \dots, \mathbf{x}_{1n_1}, \mathbf{x}_{21}, \dots, \mathbf{x}_{2n_2})$. Let $t_j = -1$ for $j = 1, \dots, n_1$ and $t_j = 1$ for $j = n_1 + 1, \dots, N$. By differentiating the Lagrangian formulation with respect to \mathbf{w} and b , we obtain the following dual form:

$$L(\boldsymbol{\alpha}) = \sum_{j=1}^N \alpha_j - \frac{1}{2} \sum_{j=1}^N \sum_{j'=1}^N \alpha_j \alpha_{j'} t_j t_{j'} k(\mathbf{x}_j, \mathbf{x}_{j'}),$$

where $k(\mathbf{x}_j, \mathbf{x}_{j'}) = \phi(\mathbf{x}_j)^T \phi(\mathbf{x}_{j'})$ is a kernel function, and $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_N)^T$ and α_j s are Lagrange multipliers such as $\mathbf{w} = \sum_{j=1}^N \alpha_j t_j \phi(\mathbf{x}_j)$. The optimization problem can be transformed into the following: $\operatorname{argmax}_{\boldsymbol{\alpha}} L(\boldsymbol{\alpha})$ subject to

$$\alpha_j \geq 0, \quad j = 1, \dots, N, \quad \text{and} \quad \sum_{j=1}^N \alpha_j t_j = 0. \quad (2)$$

Let us write that

$$\hat{\boldsymbol{\alpha}} = (\hat{\alpha}_1, \dots, \hat{\alpha}_N)^T = \operatorname{argmax}_{\boldsymbol{\alpha}} L(\boldsymbol{\alpha}) \quad \text{subject to (2)}.$$

There exist some \mathbf{x}_j s satisfying that $t_j y(\mathbf{x}_j) = 1$ (i.e., $\hat{\alpha}_j \neq 0$). Such \mathbf{x}_j s are called the support vector. Let $\hat{S} = \{j | \hat{\alpha}_j \neq 0, j = 1, \dots, N\}$ and $N_{\hat{S}} = \#\hat{S}$, where $\#A$ denotes the number of

elements in a set A . The intercept term is given by $\hat{b} = N_{\hat{S}}^{-1} \sum_{j \in \hat{S}} \{t_j - \sum_{j' \in \hat{S}} \hat{\alpha}_{j'} t_{j'} k(\mathbf{x}_j, \mathbf{x}_{j'})\}$. Then, the classifier in (1) is defined by

$$\hat{y}(\mathbf{x}) = \sum_{j \in \hat{S}} \hat{\alpha}_j t_j k(\mathbf{x}, \mathbf{x}_j) + \hat{b}. \quad (3)$$

Finally, in SVM, one classifies \mathbf{x}_0 into Π_1 if $\hat{y}(\mathbf{x}_0) < 0$ and into Π_2 otherwise. See Vapnik [14] for the details. Let $e(i)$ denote the error rate of misclassifying an individual from Π_i into the other class for $i = 1, 2$. We claim that a classifier has consistency if

$$e(i) = o(1) \text{ as } d \rightarrow \infty \text{ for } i = 1, 2. \quad (4)$$

In this paper, we investigate the following typical kernels.

- (I) The linear kernel: $k(\mathbf{x}_j, \mathbf{x}_{j'}) = \mathbf{x}_j^T \mathbf{x}_{j'}$; and
 (II) The Gaussian kernel: $k(\mathbf{x}_j, \mathbf{x}_{j'}) = \exp(-\|\mathbf{x}_j - \mathbf{x}_{j'}\|^2 / \gamma)$,

where $\gamma(> 0)$ is a scale parameter.

2.2 Asymptotic properties of SVM

First, we assume the following assumption as $d \rightarrow \infty$:

(A-i) $k(\mathbf{x}_{1j}, \mathbf{x}_{1j'}) = \beta_1 + o_P(\Delta)$ for all $1 \leq j < j' \leq n_1$;

$$k(\mathbf{x}_{1j}, \mathbf{x}_{1j}) = \beta_2 + o_P(\Delta) \text{ for all } 1 \leq j \leq n_1;$$

$$k(\mathbf{x}_{2j}, \mathbf{x}_{2j'}) = \beta_3 + o_P(\Delta) \text{ for all } 1 \leq j < j' \leq n_2;$$

$$k(\mathbf{x}_{2j}, \mathbf{x}_{2j}) = \beta_4 + o_P(\Delta) \text{ for all } 1 \leq j \leq n_2; \text{ and}$$

$$k(\mathbf{x}_{1j}, \mathbf{x}_{2j'}) = \beta_5 + o_P(\Delta) \text{ for all } 1 \leq j \leq n_1, 1 \leq j' \leq n_2;$$

$$k(\mathbf{x}_0, \mathbf{x}_{ij}) = \beta_{2i-1} + o_P(\Delta) \text{ when } \mathbf{x}_0 \in \Pi_i \text{ for all } 1 \leq j \leq n_i \text{ and } i = 1, 2;$$

$$k(\mathbf{x}_0, \mathbf{x}_{i'j}) = \beta_5 + o_P(\Delta) \text{ when } \mathbf{x}_0 \in \Pi_i \text{ for all } 1 \leq j \leq n_{i'} \text{ and } i' \neq i.$$

Here, β_l is a variable (which may depend on d) for $l = 1, \dots, 5$ and $\Delta = \beta_1 + \beta_3 - 2\beta_5$, where $\Delta > 0$, $\beta_2 - \beta_1 \geq 0$ and $\beta_4 - \beta_3 \geq 0$.

We note that Δ is a distance between the two populations. For example, $\Delta = \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\|^2$ when $k(\cdot, \cdot)$ is the linear kernel. See Section 3.1 for the details. Let $\eta_1 = \beta_2 - \beta_1$ and $\eta_2 = \beta_4 - \beta_3$. We note that $\sum_{j=1}^{n_1} \alpha_j = \sum_{j=n_1+1}^N \alpha_j$ ($= \alpha_*$, say) under (2). Then, from Section 2 of Nakayama et al. [11], we have the following lemma.

Lemma 1 ([11]). *Under (2) and (A-i), it holds that as $d \rightarrow \infty$*

$$L(\boldsymbol{\alpha}) = 2\alpha_* - \frac{\Delta}{2}\alpha_*^2 - \frac{1}{2} \left(\eta_1 \sum_{j=1}^{n_1} \alpha_j^2 + \eta_2 \sum_{j=n_1+1}^N \alpha_j^2 \right) + o_P(\Delta \alpha_*^2).$$

We can claim that

$$\max_{\alpha} \left\{ -\frac{1}{2} \left(\eta_1 \sum_{j=1}^{n_1} \alpha_j^2 + \eta_2 \sum_{j=n_1+1}^N \alpha_j^2 \right) \right\} = -\frac{\alpha_*^2}{2} (\eta_1/n_1 + \eta_2/n_2)$$

when $\alpha_1 = \dots = \alpha_{n_1} = \alpha_*/n_1$ and $\alpha_{n_1+1} = \dots = \alpha_N = \alpha_*/n_2$ under (2). Let $\Delta_* = \Delta + \eta_1/n_1 + \eta_2/n_2$. We consider the following condition:

$$\liminf_{d \rightarrow \infty} \frac{\eta_i}{\Delta} > 0 \text{ for } i = 1, 2. \quad (5)$$

Then, in a way similar to Section 2 of Nakayama et al. [9], from Lemma 1 it holds that

$$\max_{\alpha} L(\alpha) = -\frac{\Delta_*}{2} \left(\alpha_* - \frac{2 + o_P(1)}{\Delta_*} \right)^2 \{1 + o_P(1)\} + \frac{2 + o_P(1)}{\Delta_*} \quad (6)$$

under (2), (5) and (A-i), so that $\alpha_* \approx 2/\Delta_*$. Then, from (6), we have the following result.

Proposition 1 ([11]). *Let $\delta = \eta_1/n_1 - \eta_2/n_2$. Assume (A-i) and (5). It holds that as $d \rightarrow \infty$*

$$\begin{aligned} \hat{\alpha}_j &= \frac{2}{\Delta_* n_1} \{1 + o_P(1)\} \text{ for all } j = 1, \dots, n_1; \text{ and} \\ \hat{\alpha}_j &= \frac{2}{\Delta_* n_2} \{1 + o_P(1)\} \text{ for all } j = n_1 + 1, \dots, N. \end{aligned}$$

Furthermore, it holds that as $d \rightarrow \infty$

$$\hat{y}(\mathbf{x}_0) = \frac{\Delta}{\Delta_*} \left((-1)^i + \frac{\delta}{\Delta} + o_P(1) \right) \text{ when } \mathbf{x}_0 \in \Pi_i \text{ for } i = 1, 2.$$

Now, we consider the following condition:

$$\text{(C-i)} \quad \limsup_{d \rightarrow \infty} \frac{|\delta|}{\Delta} < 1.$$

For the misclassification rates, from Section 2 of Nakayama et al. [11], we have the following results.

Theorem 1 ([11]). *Under (A-i) and (C-i), SVM (3) holds consistency (4).*

Corollary 1 ([11]). *Under (A-i), SVM (3) holds the following properties:*

$$e(1) = 1 + o(1) \text{ and } e(2) = o(1) \text{ as } d \rightarrow \infty \quad (7)$$

$$\text{if } \liminf_{d \rightarrow \infty} \frac{\delta}{\Delta} > 1; \text{ and}$$

$$e(1) = o(1) \text{ and } e(2) = 1 + o(1) \text{ as } d \rightarrow \infty \quad (8)$$

$$\text{if } \limsup_{d \rightarrow \infty} \frac{\delta}{\Delta} < -1.$$

For linear SVM, Nakayama et al. [9] showed consistency (4) and the results in Corollary 1. From Corollary 1, if $|\delta|$ is larger than Δ , SVM would give a bad performance. Nakayama et al. [11] proposed a robust SVM in HDLSS settings.

3 Asymptotic properties of SVM with kernel functions (I) or (II)

We assume that $\limsup_{d \rightarrow \infty} \|\boldsymbol{\mu}_i\|^2/d < \infty$ and $\text{tr}(\boldsymbol{\Sigma}_i)/d \in (0, \infty)$ as $d \rightarrow \infty$ for $i = 1, 2$. Here, for a function, $f(\cdot)$, “ $f(d) \in (0, \infty)$ as $d \rightarrow \infty$ ” implies $\liminf_{d \rightarrow \infty} f(d) > 0$ and $\limsup_{d \rightarrow \infty} f(d) < \infty$. Similar to Aoshima and Yata [2], we assume the following assumption for Π_i s as necessary:

(A-ii) Let \mathbf{z}_{ij} , $j = 1, \dots, n_i$, be i.i.d. random p_i -vectors having $E(\mathbf{z}_{ij}) = \mathbf{0}$ and $\text{Var}(\mathbf{z}_{ij}) = \mathbf{I}_{p_i}$ for each $i (= 1, 2)$ and some p_i . Let $\mathbf{z}_{ij} = (z_{i1j}, \dots, z_{ip_i j})^\top$ whose components satisfy that $\limsup_{d \rightarrow \infty} E(z_{irj}^4) < \infty$ for all r and

$$E(z_{irj}^2 z_{isj}^2) = E(z_{irj}^2) E(z_{isj}^2) = 1 \quad \text{and} \quad E(z_{irj} z_{isj} z_{itj} z_{iu j}) = 0$$

for all $r \neq s, t, u$. Then, the observations, \mathbf{x}_{ij} s, from each Π_i ($i = 1, 2$) are given by $\mathbf{x}_{ij} = \boldsymbol{\Gamma}_i \mathbf{z}_{ij} + \boldsymbol{\mu}_i$, $j = 1, \dots, n_i$, where $\boldsymbol{\Gamma}_i$ is a $d \times p_i$ matrix such that $\boldsymbol{\Gamma}_i \boldsymbol{\Gamma}_i^\top = \boldsymbol{\Sigma}_i$.

Note that \mathbf{z}_{irj} s are i.i.d. as the standard normal distribution when the Π_i s are Gaussian and $\boldsymbol{\Gamma}_i = \mathbf{H}_i \boldsymbol{\Lambda}_i^{1/2}$, where $\boldsymbol{\Lambda}_i = \text{diag}(\lambda_{i(1)}, \dots, \lambda_{i(d)})$ is a diagonal matrix of eigenvalues, $\lambda_{i(1)} \geq \dots \geq \lambda_{i(d)} \geq 0$, and \mathbf{H}_i is an orthogonal matrix of the corresponding eigenvectors. Thus, (A-ii) naturally holds when the Π_i s are Gaussian.

3.1 Linear kernel function (I)

We consider linear SVM (LSVM), that is, the classifier (3) having kernel function (I). We set $\beta_1 = \|\boldsymbol{\mu}_1\|^2$, $\beta_2 = \|\boldsymbol{\mu}_1\|^2 + \text{tr}(\boldsymbol{\Sigma}_1)$, $\beta_3 = \|\boldsymbol{\mu}_2\|^2$, $\beta_4 = \|\boldsymbol{\mu}_2\|^2 + \text{tr}(\boldsymbol{\Sigma}_2)$ and $\beta_5 = \boldsymbol{\mu}_1^\top \boldsymbol{\mu}_2$, so that

$$\Delta = \|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\|^2 (= \Delta_{(I)}, \text{ say}) \quad \text{and} \quad \eta_i = \text{tr}(\boldsymbol{\Sigma}_i) (= \eta_{i(I)}, \text{ say}) \quad \text{for } i = 1, 2.$$

We note that LSVM is invariant to linear transformations on the data set. Thus, in Section 3.1, we assume $\boldsymbol{\mu}_2 = \mathbf{0}$ without loss of generality, so that $\beta_3 = \beta_5 = 0$, $\beta_4 = \eta_{2(I)}$ and $\Delta_{(I)} = \|\boldsymbol{\mu}_1\|^2$. In addition, we assume the following condition as $d \rightarrow \infty$:

(C-ii) $\frac{\text{tr}(\boldsymbol{\Sigma}_i^2)}{\Delta_{(I)}^2} = o(1)$ for $i = 1, 2$.

Then, from Section 3 of Nakayama et al. [11], we have the following lemma.

Lemma 2 ([11]). *Assume (A-ii) and (C-ii). Then, the assumption (A-i) is met for kernel function (I).*

By combining Lemma 2 with Theorem 1 and Corollary 1, we have the following results.

Corollary 2. *For LSVM, one can claim that*

$$(4) \text{ holds if } \limsup_{d \rightarrow \infty} \frac{|\delta_{(I)}|}{\Delta_{(I)}} < 1; \quad (7) \text{ holds if } \liminf_{d \rightarrow \infty} \frac{\delta_{(I)}}{\Delta_{(I)}} > 1; \quad \text{and}$$

$$(8) \text{ holds if } \limsup_{d \rightarrow \infty} \frac{\delta_{(I)}}{\Delta_{(I)}} < -1$$

under (A-ii) and (C-ii), where $\delta_{(I)} = \eta_{1(I)}/n_1 - \eta_{2(I)}/n_2$.

Nakayama et al. [9] provided a bias correction of linear SVM (BC-LSVM). They compared BC-LSVM with LSVM both in numerical simulations and actual data analyses. They concluded that BC-LSVM gives adequate performances for HDLSS settings even when n_i s are quite unbalanced.

3.2 Gaussian kernel function (II)

We consider Gaussian kernel SVM (GSVM), that is, the classifier (3) with kernel function (II). We set $\beta_1 = \exp\{-2\text{tr}(\mathbf{\Sigma}_1)/\gamma\}$ ($= \beta_{1(II)}$, say), $\beta_3 = \exp\{-2\text{tr}(\mathbf{\Sigma}_2)/\gamma\}$ ($= \beta_{3(II)}$, say), $\beta_2 = \beta_4 = 1$, and $\beta_5 = \exp[-\{\text{tr}(\mathbf{\Sigma}_1) + \text{tr}(\mathbf{\Sigma}_2) + \Delta_{(I)}\}/\gamma]$ ($= \beta_{5(II)}$, say), so that

$$\Delta = \beta_{1(II)} + \beta_{3(II)} - 2\beta_{5(II)} \quad (= \Delta_{(II)}, \text{ say}) \quad \text{and}$$

$$\eta_i = 1 - \exp(-2\text{tr}(\mathbf{\Sigma}_i)/\gamma) \quad (= \eta_{i(II)}, \text{ say}) \quad \text{for } i = 1, 2.$$

We note that $\Delta_{(II)} > 0$ when $\boldsymbol{\mu}_1 \neq \boldsymbol{\mu}_2$ or $\text{tr}(\mathbf{\Sigma}_1) \neq \text{tr}(\mathbf{\Sigma}_2)$. Let $\text{tr}(\mathbf{\Sigma}_{\min}) = \min_{i=1,2} \text{tr}(\mathbf{\Sigma}_i)$ and $\psi = \exp\{-2\text{tr}(\mathbf{\Sigma}_{\min})/\gamma\}$. We assume the following condition as $d \rightarrow \infty$:

$$(C\text{-iii}) \quad \frac{\text{tr}(\mathbf{\Sigma}_i^2) + \Delta_{(I)}\{\text{tr}(\mathbf{\Sigma}_i^2)\}^{1/2}}{\min\{\gamma^2\Delta_{(II)}^2/\psi^2, \gamma^2\}} = o(1) \quad \text{for } i = 1, 2.$$

Then, from Section 3 of Nakayama et al. [11], we have the following lemma.

Lemma 3 ([11]). *Assume (A-ii) and (C-iii). Then, the assumption (A-i) is met for kernel function (II).*

By combining Lemma 3 with Theorem 1 and Corollary 1, we have the following results.

Corollary 3. *For GSVM, one can claim that*

$$(4) \text{ holds if } \limsup_{d \rightarrow \infty} \frac{|\delta_{(II)}|}{\Delta_{(II)}} < 1; \quad (7) \text{ holds if } \liminf_{d \rightarrow \infty} \frac{\delta_{(II)}}{\Delta_{(II)}} > 1; \quad \text{and}$$

$$(8) \text{ holds if } \limsup_{d \rightarrow \infty} \frac{\delta_{(II)}}{\Delta_{(II)}} < -1$$

under (A-ii) and (C-iii), where $\delta_{(II)} = \eta_{1(II)}/n_1 - \eta_{2(II)}/n_2$.

Nakayama et al. [11] provided a bias correction of GSVM (BC-GSVM). They compared BC-GSVM with GSVM both in numerical simulations and actual data analyses. They also discussed the choice of γ .

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